

1,3-Dioxolane  
646-06-0 | DTXSID4027284

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 65.9 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.42e-01

Confidence level: 7.97e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Ethyl-2-hexenal</div> <div>Measured: 79.0</div> <div>Predicted: 1.35</div>	<div>Image not found</div> <div>Butyl acetate</div> <div>Measured: 38.1</div> <div>Predicted: 16.4</div>	<div>Image not found</div> <div>2-Butyne-1,4-diol</div> <div>Measured: 48.0</div> <div>Predicted: 2.85e-03</div>
<div>Image not found</div> <div>Fluorobenzene</div> <div>Measured: 34.1</div> <div>Predicted: 58.3</div>	<div>Image not found</div> <div>1,2,3,5-Tetramethylbenzene</div> <div>Measured: 171</div> <div>Predicted: 7.40e-01</div>	